π-$FeMg_3Al_8Si_6$ ($E9_b$) Structure: A8BC3D6_hP18_189_agh_b_f_i-001

This structure previously used the label(s) `A8BC3D6_hP18_189_bfh_a_g_i`. Calls to these addresses will be redirected here.

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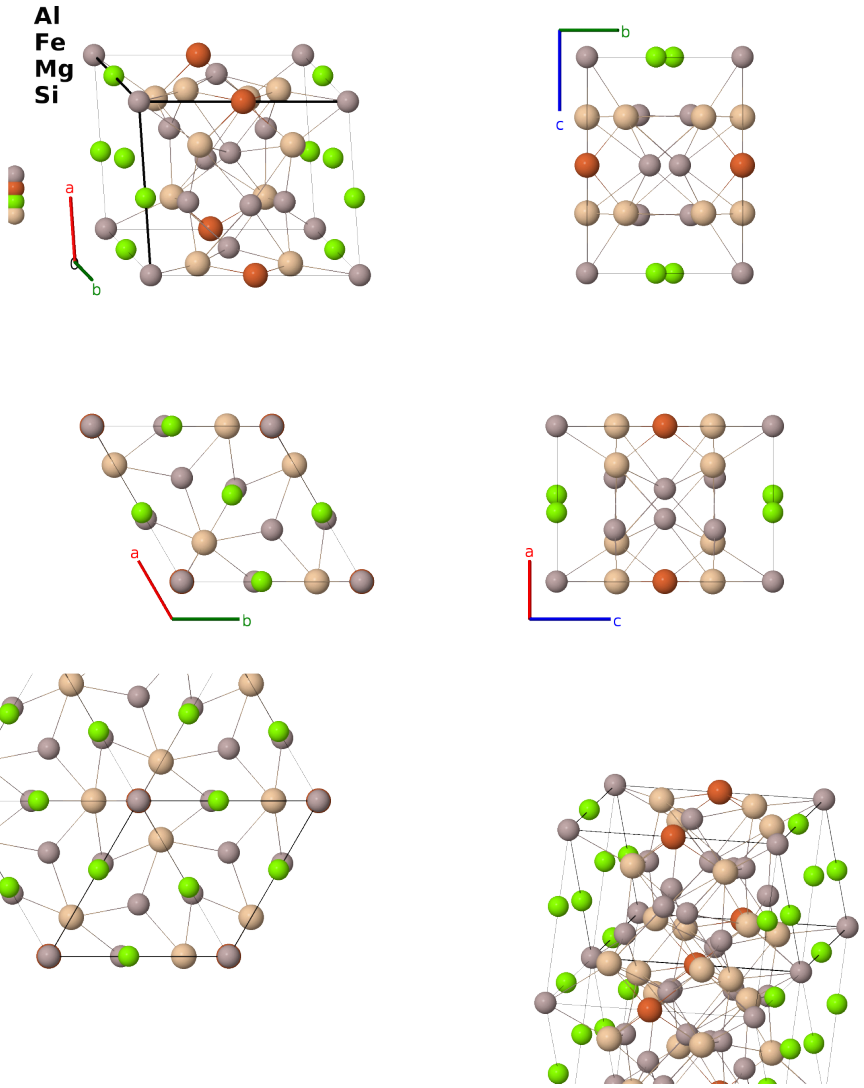
https://aflow.org/prototype-encyclopedia/WS3B

https://aflow.org/prototype-encyclopedia/A8BC3D6_hP18_189_agh_b_f_i-001



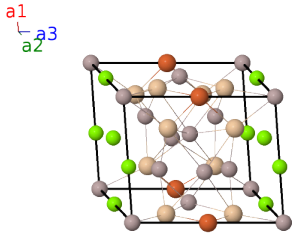
Prototype	$Al_8FeMg_3Si_6$
AFLOW prototype label	A8BC3D6_hP18_189_agh_b_f_i-001
***Strukturbericht* designation**	$E9_b$

ICSD	21740
CCDC	1829560
Pearson symbol	hP18
Space group number	189
Space group symbol	$P\bar{6}2m$
AFLOW prototype command	`aflow --proto=A8BC3D6_hP18_189_agh_b_f_i-001 --params=`$a, c/a, x_3, x_4, z_5, x_6, z_6$

- We have been unable to obtain a copy of (Perlitz, 1942), and use the data provided by (Brandes, 1992) and (Foss, 2003). Foss et al. argue that the actual composition of this phase should be $FeMg_3Al_9Si_5$. This requires a reordering of the atomic positions, as described in A9BC3D5_hP18_189_fi_a_g_bh.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Fe I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	Mg I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_2$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	Mg I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(3f)	Mg I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Al II
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Al II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Al II
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4h)	Al III
$\mathbf{B_{10}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4h)	Al III
$\mathbf{B_{11}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4h)	Al III
$\mathbf{B_{12}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4h)	Al III
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6i)	Si I
$\mathbf{B_{14}}$	=	$x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6i)	Si I
$\mathbf{B_{15}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(6i)	Si I
$\mathbf{B_{16}}$	=	$x_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6i)	Si I

$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6i)	Si I
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - cz_6\,\hat{\mathbf{z}}$	(6i)	Si I

References

[1] H. Perlitz and A. Westgren, *The Crystal Structure of $Al_8Si_6Mg_3Fe$*, Ark. Kemi Mineral. Geol. **15B**, 1–8 (1942).

[2] E. A. Brandes and G. B. Brook, eds., *Smithells Metals Reference Book* (Butterworth Heinemann, Oxford, Auckland, Boston, Johannesburg, Melbourne, New Delhi, 1992), chap. 6, pp. 6–60, seventh edn.

Found in

[1] S. Foss, A. Olsen, C. J. Simensen, and J. Tafto, *Determination of the crystal structure of the π-AlFeMgSi phase using symmetry- and site-sensitive electron microscope techniques*, Acta Crystallogr. Sect. B **59**, 36–42 (2003), doi:10.1107/S0108768102022887.

First cited in

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